



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:17 PM UTC

PDB ID : 1TDA / pdb_00001tda
Title : STRUCTURES OF THYMIDYLATE SYNTHASE WITH A C-TERMINAL DELETION: ROLE OF THE C-TERMINUS IN ALIGNMENT OF D/UMP AND CH₂H₄FOLATE
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Deposited on : 1993-02-15
Resolution : 3.09 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

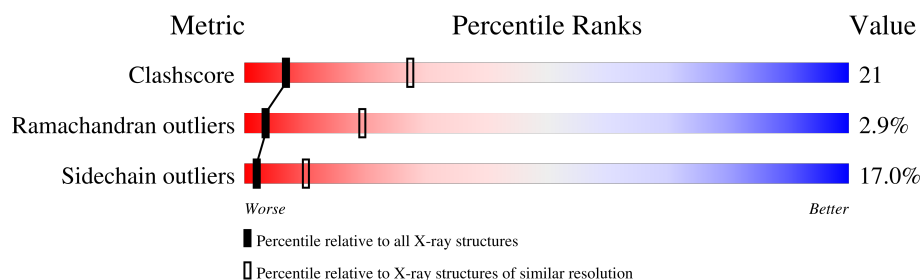
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	315	24% 40% 30% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	317	-	X	-	-

2 Entry composition [i](#)

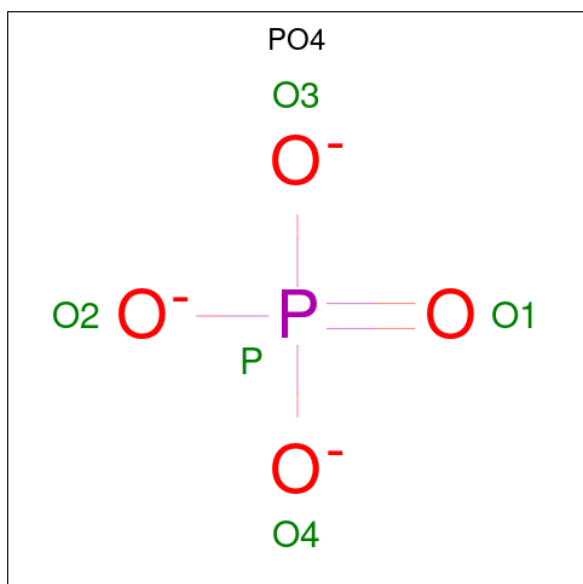
There are 3 unique types of molecules in this entry. The entry contains 2641 atoms, of which 0 are hydrogens and 16 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called THYMIDYLATE SYNTHASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	D	N	O	S			
1	A	315	2599	1672	16	437	466	8	0	0	0

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	5	4	1	0	0

- Molecule 3 is water.

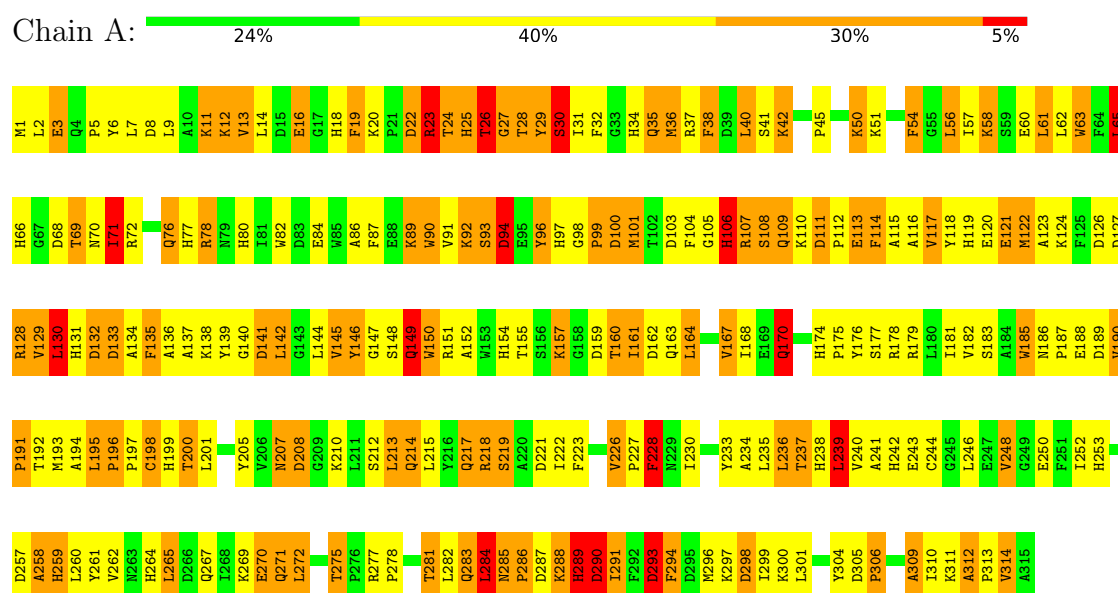
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	37	37	37	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: THYMIDYLATE SYNTHASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	78.80Å 78.80Å 243.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 3.09	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.09)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.160 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2641	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.47	78/2667 (2.9%)	2.84	284/3624 (7.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	THR	C-N	46.31	1.92	1.33
1	A	108	SER	C-N	42.63	1.92	1.33
1	A	114	PHE	C-N	42.58	1.93	1.33
1	A	19	PHE	C-N	-13.97	1.13	1.33
1	A	192	THR	CA-CB	12.39	1.72	1.53
1	A	66	HIS	CG-ND1	-10.05	1.27	1.38
1	A	117	VAL	CA-CB	9.15	1.64	1.54
1	A	219	SER	CA-CB	-8.62	1.38	1.53
1	A	199	HIS	CG-ND1	-8.19	1.29	1.38
1	A	199	HIS	CD2-NE2	-7.96	1.29	1.37
1	A	264	HIS	CD2-NE2	-7.91	1.29	1.37
1	A	77	HIS	CD2-NE2	-7.82	1.29	1.37
1	A	80	HIS	CG-ND1	-7.62	1.29	1.38
1	A	259	HIS	CD2-NE2	-7.51	1.29	1.37
1	A	94	ASP	N-CA	7.49	1.55	1.46
1	A	100	ASP	CA-C	7.29	1.62	1.52
1	A	97	HIS	CA-CB	7.27	1.61	1.53
1	A	18	HIS	CG-ND1	-7.24	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	137	ALA	CA-CB	-7.24	1.42	1.53
1	A	253	HIS	CD2-NE2	-7.15	1.29	1.37
1	A	238	HIS	CG-ND1	-7.10	1.30	1.38
1	A	187	PRO	CA-CB	-7.07	1.43	1.53
1	A	267	GLN	CA-CB	-6.80	1.42	1.53
1	A	289	HIS	CG-CD2	6.76	1.43	1.35
1	A	25	HIS	CB-CG	6.74	1.59	1.50
1	A	264	HIS	CG-ND1	-6.71	1.30	1.38
1	A	80	HIS	CD2-NE2	-6.68	1.30	1.37
1	A	196	PRO	CA-CB	-6.59	1.45	1.54
1	A	93	SER	N-CA	6.58	1.54	1.45
1	A	78	ARG	NE-CZ	6.41	1.40	1.33
1	A	293	ASP	CA-CB	-6.27	1.44	1.53
1	A	150	TRP	NE1-CE2	-6.26	1.30	1.37
1	A	18	HIS	CD2-NE2	-6.25	1.30	1.37
1	A	82	TRP	NE1-CE2	-6.15	1.30	1.37
1	A	195	LEU	CA-CB	6.03	1.61	1.53
1	A	132	ASP	CA-CB	5.98	1.61	1.52
1	A	309	ALA	CA-CB	-5.97	1.43	1.53
1	A	82	TRP	CG-CD2	-5.97	1.33	1.43
1	A	100	ASP	C-N	5.94	1.41	1.33
1	A	154	HIS	CA-C	-5.90	1.45	1.52
1	A	63	TRP	NE1-CE2	-5.85	1.31	1.37
1	A	66	HIS	CD2-NE2	-5.84	1.31	1.37
1	A	213	LEU	CB-CG	-5.80	1.41	1.53
1	A	267	GLN	N-CA	-5.79	1.39	1.46
1	A	154	HIS	CD2-NE2	-5.79	1.31	1.37
1	A	22	ASP	N-CA	5.78	1.53	1.46
1	A	196	PRO	N-CD	-5.76	1.39	1.47
1	A	131	HIS	CG-CD2	5.71	1.42	1.35
1	A	69	THR	CA-CB	-5.70	1.44	1.53
1	A	290	ASP	C-N	5.70	1.40	1.33
1	A	92	LYS	N-CA	5.69	1.52	1.46
1	A	242	HIS	CD2-NE2	-5.67	1.31	1.37
1	A	246	LEU	CB-CG	-5.63	1.42	1.53
1	A	45	PRO	CA-CB	-5.62	1.50	1.53
1	A	298	ASP	C-N	5.61	1.40	1.33
1	A	293	ASP	N-CA	-5.57	1.39	1.46
1	A	191	PRO	CA-CB	-5.52	1.46	1.53
1	A	8	ASP	CA-CB	-5.52	1.44	1.53
1	A	45	PRO	C-N	-5.46	1.25	1.33
1	A	246	LEU	CA-CB	-5.46	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	200	THR	CA-CB	-5.42	1.45	1.53
1	A	131	HIS	CD2-NE2	-5.40	1.31	1.37
1	A	34	HIS	CG-ND1	-5.36	1.32	1.38
1	A	191	PRO	N-CA	-5.35	1.40	1.47
1	A	146	TYR	C-O	-5.32	1.17	1.24
1	A	94	ASP	CA-C	5.29	1.59	1.52
1	A	63	TRP	CG-CD2	-5.27	1.34	1.43
1	A	131	HIS	CB-CG	5.26	1.57	1.50
1	A	8	ASP	N-CA	-5.21	1.40	1.46
1	A	242	HIS	CG-ND1	-5.18	1.32	1.38
1	A	313	PRO	C-O	5.17	1.29	1.23
1	A	238	HIS	CD2-NE2	-5.11	1.32	1.37
1	A	56	LEU	CA-CB	5.09	1.62	1.53
1	A	282	LEU	CA-CB	-5.06	1.46	1.53
1	A	138	LYS	CA-CB	5.04	1.61	1.53
1	A	240	VAL	CA-CB	-5.03	1.47	1.54
1	A	90	TRP	NE1-CE2	-5.03	1.31	1.37
1	A	119	HIS	CG-CD2	5.00	1.41	1.35

All (284) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	THR	O-C-N	-20.03	95.95	122.59
1	A	108	SER	O-C-N	-16.18	100.13	122.46
1	A	108	SER	CA-C-N	14.67	153.49	121.80
1	A	108	SER	C-N-CA	14.67	153.49	121.80
1	A	174	HIS	CA-CB-CG	-14.38	99.42	113.80
1	A	114	PHE	O-C-N	-14.11	106.12	122.20
1	A	218	ARG	N-CA-C	12.89	128.27	112.54
1	A	214	GLN	OE1-CD-NE2	-12.81	109.79	122.60
1	A	290	ASP	CA-CB-CG	12.49	125.09	112.60
1	A	76	GLN	OE1-CD-NE2	-12.47	110.12	122.60
1	A	189	ASP	CA-CB-CG	12.34	124.94	112.60
1	A	221	ASP	CA-CB-CG	12.18	124.78	112.60
1	A	114	PHE	CA-C-N	11.87	144.21	121.54
1	A	114	PHE	C-N-CA	11.87	144.21	121.54
1	A	193	MET	N-CA-C	11.59	125.61	110.43
1	A	54	PHE	CA-C-O	-10.81	108.95	120.63
1	A	228	PHE	CA-CB-CG	10.20	124.00	113.80
1	A	192	THR	N-CA-C	-9.84	100.11	111.03
1	A	77	HIS	CB-CG-CD2	-9.82	118.44	131.20
1	A	200	THR	N-CA-C	9.79	121.64	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	ASP	CA-CB-CG	9.65	122.25	112.60
1	A	24	THR	O-C-N	9.60	135.05	122.19
1	A	6	TYR	O-C-N	9.40	132.18	122.03
1	A	122	MET	CA-C-O	-9.40	110.49	120.55
1	A	122	MET	N-CA-C	-9.02	100.39	111.40
1	A	271	GLN	OE1-CD-NE2	-8.94	113.66	122.60
1	A	214	GLN	CG-CD-NE2	8.74	129.51	116.40
1	A	149	GLN	CG-CD-NE2	-8.73	103.31	116.40
1	A	241	ALA	N-CA-C	-8.67	101.78	111.14
1	A	24	THR	N-CA-C	-8.64	99.64	111.56
1	A	154	HIS	CA-CB-CG	-8.53	105.27	113.80
1	A	170	GLN	OE1-CD-NE2	-8.47	114.13	122.60
1	A	109	GLN	N-CA-C	-8.44	99.88	112.04
1	A	84	GLU	CA-CB-CG	-8.42	97.25	114.10
1	A	219	SER	CA-CB-OG	-8.37	94.37	111.10
1	A	175	PRO	N-CA-C	-8.36	103.41	113.86
1	A	177	SER	CA-C-O	8.31	130.48	120.92
1	A	82	TRP	N-CA-C	8.26	124.46	113.72
1	A	261	TYR	CA-C-O	-8.07	112.19	121.72
1	A	133	ASP	O-C-N	8.05	131.37	122.11
1	A	108	SER	N-CA-C	-8.03	103.38	113.01
1	A	185	TRP	N-CA-C	8.00	120.67	109.15
1	A	160	THR	CA-CB-OG1	-7.94	97.69	109.60
1	A	283	GLN	CB-CG-CD	-7.88	99.20	112.60
1	A	106	HIS	N-CA-CB	7.87	123.80	110.49
1	A	290	ASP	CA-C-O	-7.86	112.46	121.66
1	A	82	TRP	CA-C-O	7.85	127.69	119.05
1	A	100	ASP	CA-CB-CG	7.85	120.45	112.60
1	A	61	LEU	CA-C-O	-7.85	112.10	120.42
1	A	130	LEU	N-CA-C	7.84	120.72	111.71
1	A	80	HIS	CB-CG-CD2	-7.83	121.02	131.20
1	A	194	ALA	N-CA-C	7.80	119.41	111.07
1	A	170	GLN	CG-CD-NE2	7.78	128.07	116.40
1	A	116	ALA	N-CA-C	7.78	121.87	112.38
1	A	24	THR	CB-CA-C	7.73	123.25	111.18
1	A	147	GLY	CA-C-O	7.72	128.74	120.40
1	A	119	HIS	CB-CG-CD2	-7.71	121.18	131.20
1	A	62	LEU	CA-C-N	7.69	130.89	120.44
1	A	62	LEU	C-N-CA	7.69	130.89	120.44
1	A	154	HIS	CB-CG-CD2	-7.66	121.24	131.20
1	A	277	ARG	CA-C-N	7.62	128.08	119.93
1	A	277	ARG	C-N-CA	7.62	128.08	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	LEU	N-CA-C	-7.61	101.42	111.24
1	A	217	GLN	OE1-CD-NE2	-7.52	115.08	122.60
1	A	258	ALA	CA-C-O	-7.50	112.43	121.28
1	A	160	THR	CA-CB-CG2	7.49	123.24	110.50
1	A	272	LEU	O-C-N	-7.46	113.49	122.22
1	A	84	GLU	O-C-N	7.38	129.95	122.12
1	A	120	GLU	N-CA-C	-7.25	102.36	112.45
1	A	8	ASP	N-CA-CB	-7.25	99.47	110.12
1	A	56	LEU	CD1-CG-CD2	-7.22	94.91	110.80
1	A	178	ARG	CB-CG-CD	-7.22	94.69	111.30
1	A	193	MET	N-CA-CB	-7.22	99.94	110.26
1	A	106	HIS	N-CA-C	-7.16	95.54	110.80
1	A	288	LYS	CA-CB-CG	-7.11	99.88	114.10
1	A	259	HIS	CA-CB-CG	7.06	120.86	113.80
1	A	63	TRP	N-CA-C	-7.01	103.57	111.14
1	A	61	LEU	N-CA-C	-6.97	103.77	111.36
1	A	121	GLU	N-CA-CB	-6.92	99.55	110.28
1	A	106	HIS	CB-CA-C	-6.92	96.65	110.42
1	A	196	PRO	N-CA-C	-6.92	102.26	110.70
1	A	304	TYR	N-CA-C	-6.92	97.28	108.41
1	A	275	THR	CB-CA-C	-6.91	101.36	110.34
1	A	193	MET	CA-C-O	6.89	129.45	121.87
1	A	170	GLN	CA-C-O	-6.88	111.67	119.79
1	A	242	HIS	CA-C-O	-6.85	113.62	120.82
1	A	26	THR	CA-C-N	6.84	129.81	120.92
1	A	26	THR	C-N-CA	6.84	129.81	120.92
1	A	305	ASP	CA-CB-CG	6.82	119.42	112.60
1	A	38	PHE	CA-C-N	-6.77	113.42	122.42
1	A	38	PHE	C-N-CA	-6.77	113.42	122.42
1	A	107	ARG	CG-CD-NE	6.77	126.89	112.00
1	A	100	ASP	N-CA-C	6.74	125.16	110.80
1	A	157	LYS	N-CA-C	6.74	122.67	113.37
1	A	76	GLN	CG-CD-NE2	6.68	126.43	116.40
1	A	77	HIS	CA-CB-CG	-6.68	107.12	113.80
1	A	250	GLU	N-CA-CB	-6.67	99.94	111.55
1	A	61	LEU	N-CA-CB	6.65	120.00	110.16
1	A	136	ALA	CA-C-N	6.64	129.51	120.54
1	A	136	ALA	C-N-CA	6.64	129.51	120.54
1	A	289	HIS	CB-CG-CD2	-6.59	122.63	131.20
1	A	109	GLN	CB-CA-C	6.59	122.62	110.56
1	A	109	GLN	N-CA-CB	-6.56	100.02	110.19
1	A	128	ARG	O-C-N	6.55	129.16	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	ARG	CA-CB-CG	6.54	127.19	114.10
1	A	149	GLN	OE1-CD-NE2	6.54	129.14	122.60
1	A	277	ARG	CB-CG-CD	-6.54	96.27	111.30
1	A	18	HIS	CB-CG-CD2	-6.53	122.71	131.20
1	A	305	ASP	CA-C-N	6.53	126.47	120.21
1	A	305	ASP	C-N-CA	6.53	126.47	120.21
1	A	13	VAL	CB-CA-C	-6.48	103.68	111.97
1	A	170	GLN	CB-CG-CD	6.48	123.61	112.60
1	A	192	THR	O-C-N	6.46	129.01	122.03
1	A	270	GLU	CA-CB-CG	6.46	127.03	114.10
1	A	192	THR	CA-C-O	-6.44	114.27	120.90
1	A	62	LEU	O-C-N	-6.43	114.03	122.39
1	A	24	THR	CA-C-N	6.41	133.79	121.54
1	A	24	THR	C-N-CA	6.41	133.79	121.54
1	A	32	PHE	CA-C-O	-6.38	113.63	120.46
1	A	214	GLN	CB-CG-CD	6.37	123.43	112.60
1	A	195	LEU	CA-C-N	6.37	126.94	120.38
1	A	195	LEU	C-N-CA	6.37	126.94	120.38
1	A	281	THR	CB-CA-C	6.34	120.20	109.80
1	A	93	SER	O-C-N	6.34	130.84	123.17
1	A	301	LEU	CD1-CG-CD2	-6.32	96.90	110.80
1	A	152	ALA	N-CA-CB	-6.31	101.91	111.19
1	A	145	VAL	O-C-N	-6.31	114.69	122.57
1	A	63	TRP	CA-CB-CG	6.30	125.57	113.60
1	A	314	VAL	N-CA-C	-6.27	100.90	109.55
1	A	260	LEU	N-CA-CB	-6.25	100.62	110.69
1	A	199	HIS	O-C-N	6.24	130.73	122.56
1	A	45	PRO	N-CA-CB	6.20	106.96	102.81
1	A	94	ASP	CA-CB-CG	-6.19	106.41	112.60
1	A	186	ASN	CB-CA-C	-6.17	103.05	110.15
1	A	133	ASP	CA-CB-CG	-6.14	106.46	112.60
1	A	313	PRO	CA-C-N	-6.11	111.84	121.62
1	A	313	PRO	C-N-CA	-6.11	111.84	121.62
1	A	22	ASP	CB-CA-C	-6.09	98.30	110.42
1	A	160	THR	N-CA-CB	-6.07	100.88	110.77
1	A	291	ILE	CA-CB-CG1	6.07	120.71	110.40
1	A	207	ASN	CA-CB-CG	6.06	118.66	112.60
1	A	141	ASP	N-CA-C	-6.04	100.01	109.25
1	A	134	ALA	CA-C-N	6.03	130.64	120.88
1	A	134	ALA	C-N-CA	6.03	130.64	120.88
1	A	118	TYR	O-C-N	-6.02	115.19	122.11
1	A	235	LEU	CA-C-O	-6.01	114.51	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	HIS	CB-CG-CD2	-6.01	123.39	131.20
1	A	183	SER	CA-CB-OG	-6.00	99.09	111.10
1	A	248	VAL	CA-C-O	6.00	127.67	120.65
1	A	144	LEU	CA-C-O	5.99	127.31	120.84
1	A	226	VAL	CG1-CB-CG2	-5.97	97.66	110.80
1	A	257	ASP	O-C-N	-5.94	115.10	122.82
1	A	42	LYS	CA-C-O	-5.92	112.91	120.31
1	A	237	THR	N-CA-C	-5.92	104.74	111.07
1	A	309	ALA	CA-C-O	-5.90	115.29	121.55
1	A	3	GLU	N-CA-C	5.90	121.52	113.37
1	A	41	SER	CA-CB-OG	5.90	122.90	111.10
1	A	178	ARG	NE-CZ-NH1	5.89	127.39	121.50
1	A	27	GLY	O-C-N	5.89	129.82	123.87
1	A	16	GLU	CA-C-O	5.89	126.32	119.32
1	A	155	THR	CA-C-O	-5.89	114.15	120.92
1	A	179	ARG	N-CA-C	-5.87	103.67	112.54
1	A	300	LYS	O-C-N	-5.87	115.77	123.16
1	A	32	PHE	CA-CB-CG	-5.86	107.94	113.80
1	A	178	ARG	NH1-CZ-NH2	-5.86	111.69	119.30
1	A	56	LEU	N-CA-C	-5.85	105.40	112.54
1	A	275	THR	OG1-CB-CG2	5.85	121.00	109.30
1	A	111	ASP	CA-C-N	5.84	127.14	119.84
1	A	111	ASP	C-N-CA	5.84	127.14	119.84
1	A	304	TYR	CA-C-O	-5.84	114.33	120.58
1	A	50	LYS	N-CA-C	-5.84	99.09	108.55
1	A	25	HIS	CB-CA-C	5.82	122.00	110.42
1	A	313	PRO	N-CA-C	5.82	121.27	111.32
1	A	35	GLN	N-CA-C	-5.81	102.16	110.59
1	A	28	THR	CA-CB-OG1	-5.81	100.89	109.60
1	A	50	LYS	CA-CB-CG	5.80	125.70	114.10
1	A	176	TYR	N-CA-CB	-5.78	102.09	110.70
1	A	96	TYR	CA-CB-CG	-5.78	103.50	113.90
1	A	198	CYS	N-CA-C	-5.76	104.37	111.40
1	A	131	HIS	N-CA-C	5.75	121.73	114.31
1	A	129	VAL	O-C-N	-5.75	116.19	121.94
1	A	281	THR	N-CA-CB	-5.75	100.67	110.16
1	A	289	HIS	CA-C-O	5.73	125.28	118.69
1	A	93	SER	CA-C-O	-5.72	114.94	121.40
1	A	271	GLN	CG-CD-NE2	5.71	124.97	116.40
1	A	199	HIS	CB-CG-CD2	-5.71	123.78	131.20
1	A	155	THR	OG1-CB-CG2	5.71	120.71	109.30
1	A	188	GLU	N-CA-C	5.70	119.41	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	LYS	CA-C-O	-5.69	111.93	119.10
1	A	54	PHE	CA-C-N	5.68	127.44	120.22
1	A	54	PHE	C-N-CA	5.68	127.44	120.22
1	A	2	LEU	CD1-CG-CD2	-5.67	98.32	110.80
1	A	108	SER	CA-CB-OG	5.67	122.44	111.10
1	A	155	THR	N-CA-C	5.65	119.45	109.96
1	A	312	ALA	O-C-N	5.65	125.89	121.88
1	A	289	HIS	CA-CB-CG	5.65	119.45	113.80
1	A	201	LEU	O-C-N	-5.63	116.52	123.33
1	A	305	ASP	O-C-N	-5.63	116.24	121.36
1	A	174	HIS	CA-C-N	5.62	125.24	119.56
1	A	174	HIS	C-N-CA	5.62	125.24	119.56
1	A	168	ILE	CA-C-O	-5.62	114.40	120.47
1	A	150	TRP	CG-CD2-CE3	5.58	139.48	133.90
1	A	13	VAL	N-CA-C	-5.58	105.06	110.42
1	A	186	ASN	CA-CB-CG	-5.57	107.03	112.60
1	A	29	TYR	CA-C-O	-5.56	114.32	120.38
1	A	301	LEU	CA-C-O	-5.56	114.14	120.32
1	A	117	VAL	CA-CB-CG2	5.53	119.80	110.40
1	A	42	LYS	N-CA-C	-5.53	104.08	112.04
1	A	135	PHE	O-C-N	5.52	128.51	122.11
1	A	147	GLY	N-CA-C	5.52	120.47	113.24
1	A	312	ALA	N-CA-C	-5.50	99.52	108.82
1	A	1	MET	N-CA-CB	5.50	119.85	110.50
1	A	182	VAL	N-CA-C	-5.50	100.57	108.48
1	A	121	GLU	CB-CG-CD	5.49	121.93	112.60
1	A	92	LYS	O-C-N	-5.48	115.64	122.11
1	A	208	ASP	N-CA-CB	-5.48	101.23	110.49
1	A	212	SER	CA-C-O	-5.47	114.97	121.16
1	A	277	ARG	O-C-N	-5.47	114.59	121.21
1	A	285	ASN	N-CA-C	5.46	121.89	109.81
1	A	164	LEU	CD1-CG-CD2	-5.45	98.82	110.80
1	A	281	THR	CA-CB-CG2	5.44	119.75	110.50
1	A	265	LEU	N-CA-C	5.42	117.94	111.71
1	A	99	PRO	N-CA-C	5.41	119.78	112.48
1	A	193	MET	CG-SD-CE	5.40	112.77	100.90
1	A	168	ILE	N-CA-C	-5.39	104.36	111.09
1	A	244	CYS	CA-CB-SG	-5.38	102.02	114.40
1	A	257	ASP	N-CA-C	5.38	117.01	108.67
1	A	230	ILE	N-CA-C	-5.34	105.17	110.62
1	A	23	ARG	O-C-N	5.33	129.67	122.59
1	A	40	LEU	N-CA-C	5.32	120.72	113.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	GLN	O-C-N	5.32	127.76	122.12
1	A	142	LEU	O-C-N	-5.32	115.17	122.46
1	A	36	MET	CA-C-O	-5.32	113.65	120.14
1	A	167	VAL	O-C-N	-5.32	116.50	121.87
1	A	284	LEU	CB-CA-C	-5.32	99.64	109.37
1	A	140	GLY	N-CA-C	-5.30	108.09	114.66
1	A	101	MET	N-CA-C	5.30	118.70	111.39
1	A	278	PRO	CA-C-O	-5.29	115.55	121.32
1	A	97	HIS	N-CA-C	-5.27	97.95	107.60
1	A	108	SER	CA-C-O	-5.27	112.20	119.05
1	A	161	ILE	CB-CA-C	-5.26	103.68	110.84
1	A	281	THR	CA-CB-OG1	-5.26	101.71	109.60
1	A	60	GLU	CB-CG-CD	5.26	121.54	112.60
1	A	259	HIS	O-C-N	5.25	129.36	123.48
1	A	5	PRO	O-C-N	5.23	129.85	122.37
1	A	283	GLN	N-CA-C	5.23	117.12	108.13
1	A	152	ALA	O-C-N	-5.23	114.46	121.78
1	A	146	TYR	N-CA-C	-5.21	105.04	111.40
1	A	80	HIS	CB-CG-ND1	5.21	130.52	122.70
1	A	199	HIS	CB-CG-ND1	5.21	130.52	122.70
1	A	37	ARG	O-C-N	-5.21	116.60	123.16
1	A	65	LEU	O-C-N	-5.18	116.63	122.12
1	A	154	HIS	CB-CG-ND1	5.18	130.47	122.70
1	A	306	PRO	O-C-N	5.17	129.27	122.86
1	A	123	ALA	CA-C-N	5.16	127.47	120.65
1	A	123	ALA	C-N-CA	5.16	127.47	120.65
1	A	262	VAL	CB-CA-C	-5.15	105.11	112.22
1	A	144	LEU	O-C-N	-5.13	116.55	122.87
1	A	12	LYS	CA-C-N	5.13	127.03	120.56
1	A	12	LYS	C-N-CA	5.13	127.03	120.56
1	A	238	HIS	O-C-N	-5.13	115.96	122.27
1	A	14	LEU	CA-C-N	-5.13	114.11	122.26
1	A	14	LEU	C-N-CA	-5.13	114.11	122.26
1	A	78	ARG	NE-CZ-NH1	5.12	126.62	121.50
1	A	27	GLY	N-CA-C	-5.11	102.81	110.38
1	A	37	ARG	NE-CZ-NH1	5.11	126.61	121.50
1	A	65	LEU	CA-C-O	-5.11	115.11	120.63
1	A	71	ILE	N-CA-CB	-5.11	103.59	110.54
1	A	131	HIS	CB-CG-CD2	-5.11	124.56	131.20
1	A	2	LEU	O-C-N	-5.10	116.72	122.03
1	A	6	TYR	CA-C-O	-5.09	115.66	120.90
1	A	210	LYS	CA-CB-CG	5.08	124.27	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	ALA	CA-C-O	-5.08	114.60	120.24
1	A	8	ASP	N-CA-C	5.08	116.81	111.28
1	A	30	SER	N-CA-C	5.08	117.69	109.06
1	A	246	LEU	N-CA-CB	5.08	118.53	110.87
1	A	286	PRO	N-CD-CG	-5.07	95.59	103.20
1	A	109	GLN	CB-CG-CD	5.07	121.21	112.60
1	A	94	ASP	N-CA-C	5.06	121.59	110.80
1	A	277	ARG	CA-C-O	-5.04	115.67	120.97
1	A	77	HIS	CB-CG-ND1	5.03	130.24	122.70
1	A	159	ASP	N-CA-C	5.02	117.62	109.79
1	A	71	ILE	CG1-CB-CG2	-5.01	95.66	110.70
1	A	294	PHE	O-C-N	5.00	128.96	123.16

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	ASP	Peptide
1	A	233	TYR	Sidechain
1	A	239	LEU	Mainchain
1	A	98	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2599	0	2483	108	0
2	A	5	0	0	0	0
3	A	37	0	0	4	0
All	All	2641	0	2483	108	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (108) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:THR:C	1:A:27:GLY:N	1.92	1.27
1:A:108:SER:C	1:A:109:GLN:N	1.92	1.26
1:A:114:PHE:C	1:A:115:ALA:N	1.93	1.25
1:A:114:PHE:O	1:A:117:VAL:HG22	1.59	1.03
1:A:107:ARG:HB3	1:A:114:PHE:CE2	1.97	0.99
1:A:290:ASP:HB2	1:A:293:ASP:HB2	1.58	0.85
1:A:107:ARG:C	1:A:114:PHE:CD2	2.60	0.81
1:A:107:ARG:C	1:A:114:PHE:HD2	1.91	0.78
1:A:57:ILE:HD11	1:A:228:PHE:HD1	1.51	0.75
1:A:71:ILE:HG22	1:A:129:VAL:HG11	1.70	0.73
1:A:92:LYS:HD2	1:A:93:SER:N	2.05	0.71
1:A:108:SER:N	1:A:114:PHE:CE2	2.59	0.71
1:A:108:SER:N	1:A:114:PHE:CD2	2.59	0.70
1:A:214:GLN:HG3	1:A:252:ILE:HB	1.73	0.70
1:A:23:ARG:NH1	1:A:24:THR:HB	2.07	0.69
1:A:94:ASP:C	1:A:96:TYR:H	2.01	0.68
1:A:63:TRP:CD1	1:A:68:ASP:HB3	2.31	0.66
1:A:92:LYS:HD2	1:A:93:SER:H	1.61	0.66
1:A:51:LYS:HB3	1:A:309:ALA:HB2	1.79	0.65
1:A:101:MET:HB3	1:A:104:PHE:HD2	1.61	0.65
1:A:126:ASP:O	1:A:130:LEU:HD22	1.96	0.64
1:A:103:ASP:HB3	1:A:106:HIS:HD2	1.63	0.63
1:A:23:ARG:HH11	1:A:24:THR:HB	1.64	0.63
1:A:222:ILE:HD11	1:A:258:ALA:HB1	1.80	0.63
1:A:54:PHE:O	1:A:57:ILE:HB	1.99	0.62
1:A:93:SER:OG	1:A:94:ASP:OD2	2.14	0.62
1:A:89:LYS:O	1:A:89:LYS:HG2	2.00	0.61
1:A:13:VAL:HG21	1:A:222:ILE:HG13	1.83	0.60
1:A:223:PHE:HE2	1:A:312:ALA:HB2	1.65	0.60
1:A:239:LEU:HG	1:A:284:LEU:HD11	1.85	0.58
1:A:72:ARG:HG2	1:A:76:GLN:HE21	1.68	0.58
1:A:94:ASP:C	1:A:96:TYR:N	2.62	0.57
1:A:198:CYS:HA	1:A:218:ARG:HG3	1.86	0.57
1:A:223:PHE:CE2	1:A:312:ALA:HB2	2.39	0.57
1:A:101:MET:HE3	1:A:117:VAL:HG23	1.88	0.55
1:A:57:ILE:HD11	1:A:228:PHE:CD1	2.39	0.55
1:A:105:GLY:O	1:A:106:HIS:ND1	2.39	0.55
1:A:146:TYR:HA	1:A:149:GLN:HE21	1.72	0.54
1:A:106:HIS:O	1:A:110:LYS:N	2.34	0.54
1:A:103:ASP:HB3	1:A:106:HIS:CD2	2.41	0.54
1:A:92:LYS:CD	1:A:93:SER:H	2.22	0.53
1:A:26:THR:O	1:A:27:GLY:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ILE:CG2	1:A:129:VAL:HG11	2.36	0.53
1:A:108:SER:N	1:A:114:PHE:HE2	2.05	0.53
1:A:197:PRO:O	1:A:218:ARG:NE	2.41	0.52
1:A:265:LEU:O	1:A:269:LYS:HB2	2.10	0.52
1:A:50:LYS:HD2	3:A:323:HOH:O	2.10	0.52
1:A:239:LEU:HG	1:A:284:LEU:CD1	2.41	0.50
1:A:108:SER:N	1:A:114:PHE:HD2	2.03	0.50
1:A:243:GLU:HG3	1:A:289:HIS:O	2.11	0.50
1:A:108:SER:CA	1:A:114:PHE:CD2	2.95	0.50
1:A:213:LEU:HD13	1:A:237:THR:OG1	2.13	0.48
1:A:127:ASP:HA	1:A:130:LEU:HD22	1.95	0.48
1:A:99:PRO:HD2	1:A:121:GLU:OE2	2.14	0.48
1:A:113:GLU:O	1:A:117:VAL:HG13	2.13	0.48
1:A:86:ALA:HB2	1:A:142:LEU:HD21	1.94	0.48
1:A:170:GLN:HE21	1:A:170:GLN:HA	1.78	0.48
1:A:196:PRO:O	1:A:218:ARG:NH2	2.48	0.47
1:A:108:SER:HA	1:A:114:PHE:CD2	2.50	0.47
1:A:291:ILE:O	1:A:294:PHE:HB2	2.15	0.47
1:A:69:THR:CG2	1:A:148:SER:HB2	2.45	0.46
1:A:70:ASN:HA	1:A:141:ASP:HA	1.97	0.46
1:A:87:PHE:CE2	1:A:122:MET:HA	2.50	0.46
1:A:132:ASP:HB3	1:A:135:PHE:CB	2.46	0.46
1:A:61:LEU:HD11	1:A:236:LEU:HG	1.97	0.45
1:A:89:LYS:O	1:A:92:LYS:CG	2.64	0.45
1:A:101:MET:HB3	1:A:104:PHE:CD2	2.47	0.45
1:A:205:TYR:HE1	1:A:207:ASN:ND2	2.15	0.45
1:A:36:MET:HE3	1:A:38:PHE:HZ	1.81	0.45
1:A:57:ILE:CD1	1:A:228:PHE:HD1	2.25	0.45
1:A:40:LEU:HD12	1:A:237:THR:HG21	1.99	0.45
1:A:12:LYS:O	1:A:16:GLU:HB2	2.17	0.45
1:A:19:PHE:HD2	1:A:29:TYR:HE1	1.63	0.45
1:A:30:SER:HB3	1:A:259:HIS:HB3	2.00	0.44
1:A:22:ASP:OD2	1:A:28:THR:OG1	2.36	0.44
1:A:185:TRP:HB3	3:A:342:HOH:O	2.18	0.44
1:A:11:LYS:HD3	3:A:337:HOH:O	2.18	0.44
1:A:151:ARG:O	1:A:162:ASP:HA	2.18	0.43
1:A:198:CYS:O	1:A:217:GLN:HA	2.19	0.43
1:A:90:TRP:C	1:A:92:LYS:H	2.26	0.43
1:A:107:ARG:CB	1:A:114:PHE:CE2	2.85	0.43
1:A:145:VAL:O	1:A:149:GLN:NE2	2.52	0.43
1:A:285:ASN:HA	1:A:286:PRO:HD3	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ILE:HG12	1:A:258:ALA:HB3	2.00	0.43
1:A:63:TRP:CH2	1:A:145:VAL:HG11	2.54	0.43
1:A:89:LYS:HE2	1:A:139:TYR:HD1	1.84	0.43
1:A:271:GLN:HB2	1:A:310:ILE:CD1	2.49	0.43
1:A:128:ARG:HB3	1:A:135:PHE:CD2	2.53	0.42
1:A:19:PHE:CZ	1:A:27:GLY:HA3	2.55	0.42
1:A:104:PHE:HA	1:A:114:PHE:CE2	2.54	0.42
1:A:50:LYS:HE3	3:A:321:HOH:O	2.19	0.42
1:A:89:LYS:O	1:A:92:LYS:HG2	2.19	0.42
1:A:145:VAL:HG12	1:A:146:TYR:H	1.85	0.42
1:A:7:LEU:HD22	1:A:272:LEU:HD23	2.02	0.42
1:A:20:LYS:HB3	1:A:22:ASP:OD2	2.20	0.42
1:A:226:VAL:N	1:A:227:PRO:HD2	2.35	0.41
1:A:51:LYS:HG3	1:A:306:PRO:HG2	2.02	0.41
1:A:149:GLN:H	1:A:149:GLN:HG2	1.64	0.41
1:A:107:ARG:C	1:A:114:PHE:CE2	2.97	0.41
1:A:150:TRP:O	1:A:163:GLN:HB3	2.21	0.41
1:A:181:ILE:HG21	1:A:181:ILE:HD13	1.89	0.41
1:A:108:SER:CA	1:A:114:PHE:HD2	2.31	0.41
1:A:288:LYS:HG2	1:A:289:HIS:N	2.36	0.41
1:A:65:LEU:O	1:A:151:ARG:NH1	2.54	0.40
1:A:108:SER:HA	1:A:114:PHE:HD2	1.86	0.40
1:A:132:ASP:HB3	1:A:135:PHE:HB2	2.02	0.40
1:A:71:ILE:HG22	1:A:129:VAL:CG1	2.45	0.40
1:A:190:VAL:HG12	1:A:191:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	313/315 (99%)	264 (84%)	40 (13%)	9 (3%)	3	19

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	ASP
1	A	112	PRO
1	A	25	HIS
1	A	94	ASP
1	A	106	HIS
1	A	26	THR
1	A	296	MET
1	A	208	ASP
1	A	190	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	276/277 (100%)	229 (83%)	47 (17%)	2 10

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	9	LEU
1	A	11	LYS
1	A	23	ARG
1	A	30	SER
1	A	35	GLN
1	A	42	LYS
1	A	56	LEU
1	A	58	LYS
1	A	65	LEU
1	A	71	ILE
1	A	78	ARG
1	A	89	LYS
1	A	91	VAL
1	A	113	GLU
1	A	124	LYS

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Mol	Chain	Res	Type
1	A	130	LEU
1	A	133	ASP
1	A	149	GLN
1	A	157	LYS
1	A	160	THR
1	A	161	ILE
1	A	164	LEU
1	A	167	VAL
1	A	170	GLN
1	A	195	LEU
1	A	200	THR
1	A	215	LEU
1	A	219	SER
1	A	228	PHE
1	A	236	LEU
1	A	239	LEU
1	A	248	VAL
1	A	270	GLU
1	A	275	THR
1	A	281	THR
1	A	283	GLN
1	A	284	LEU
1	A	287	ASP
1	A	289	HIS
1	A	290	ASP
1	A	293	ASP
1	A	297	LYS
1	A	298	ASP
1	A	299	ILE
1	A	311	LYS
1	A	314	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	106	HIS
1	A	149	GLN
1	A	170	GLN
1	A	214	GLN
1	A	289	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	A	317	-	4,4,4	2.33	2 (50%)	6,6,6	3.34	4 (66%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	317	PO4	P-O1	3.61	1.59	1.50
2	A	317	PO4	P-O4	-2.27	1.48	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	317	PO4	O4-P-O2	5.55	125.17	107.91
2	A	317	PO4	O4-P-O1	-3.53	98.47	110.95
2	A	317	PO4	O3-P-O1	-3.30	99.30	110.95
2	A	317	PO4	O2-P-O1	-2.65	101.58	110.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	114:PHE	C	115:ALA	N	1.93
1	A	26:THR	C	27:GLY	N	1.92
1	A	108:SER	C	109:GLN	N	1.92
1	A	19:PHE	C	20:LYS	N	1.13

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.